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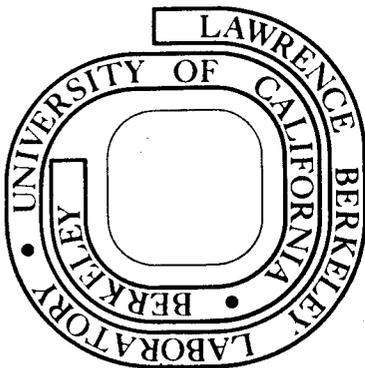
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ELASTIC SOLUTE-DISLOCATION INTERACTION
IN AN ANISOTROPIC HCP CRYSTAL

by

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ABSTRACT

The interaction due to the size misfit between a substitutional solute atom and an edge dislocation is treated employing anisotropic linear elasticity. The interaction energy contours and force-displacement relation for rigid glide of the dislocation are computed for silver and cadmium solute atoms in a zinc matrix and compared with the isotropic treatment. The results for cadmium are rather similar to those of the isotropic computation. However, for silver there are large differences in the shapes and magnitudes of the interaction energy and force relation between the isotropic and anisotropic treatments.

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I. INTRODUCTION

Solute atoms in dilute solution in a real crystal are well-known to act as localized barriers to dislocation glide. The solute atoms are often approximated as point obstacles which exert point forces on the dislocation line. This point-obstacle approximation considerably simplifies the theoretical analysis of the dislocation interaction with solute atoms. In separate reports^{1,2} we showed that the equilibrium configuration of a dislocation of edge orientation in the stress field of dilute substitutional solute atoms can be well approximated by circular bows connecting the equivalent point obstacles. We also showed that the relation of point force versus displacement of the dislocation can be reasonably well approximated by the force-displacement relation for rigid motion of a straight edge dislocation.

The force-displacement relation for the straight dislocation is customarily obtained by assuming elastic isotropy of the matrix crystal.³ But typical real crystals are elastically anisotropic. The application of anisotropy has not been fully implemented in dislocation theory because analytic expressions for dislocations on principal glide systems are unavailable or too complicated for most metals of cubic structure. However for hcp crystals an analytic solution for the dislocation stress field is available in a relatively simple form.⁴ In this report, we will utilize this result to compute the dislocation-solute interaction energy for force-displacement relation in an hcp crystal. The formulation is general. As a specific example we choose zinc as the matrix and silver and cadmium as solutes and compare with existing results obtained with an isotropic treatment.⁵

Linear elasticity is assumed sufficient to characterize dislocation behavior in the crystal. The interaction between an edge dislocation and the substitutional solute atoms is assumed due to elastic size misfit caused by the solute atoms. The interactions between solute atoms are neglected. In section 2 the interaction energies are formulated and computed. In section 3, the force-displacement relations are computed. In the last section, the relevance and validity of the present approach are discussed.

II. INTERACTION ENERGIES

The formulation of the dislocation-solute interaction is based on the assumption that the interaction is given by the elastic interaction between the stress field of the edge dislocation and the elastic size misfit associated with the substitutional solute atom. This assumption allows a straightforward derivation of expressions for the interaction.

A. Formulation

When a solute atom is substituted for a host atom in an anisotropic matrix containing an edge dislocation, the matrix is anisotropically strained against the dislocation stress field. If ϵ is the tensor strain produced by the solute atom and σ is the local tensor stress due to the dislocation, then the interaction energy, U_S , is⁶

$$U_S = - \sum_{i,j} \sigma_{ij} \epsilon_{ij} \Omega, \quad (i,j = x,y,z) \quad (1)$$

where Ω is the atomic volume of the matrix atoms.

In the coordinate system shown in Figure 1, an edge dislocation on the basal plane lies parallel to $[10\bar{1}0]$, and its Burgers vector is

parallel to $[\bar{1}2\bar{1}0]$. For this orientation the principal axes of the strain induced by a substitutional solute atom are parallel to the principal axes of the dislocation stress field. Hence Equation (1) is reduced to

$$U_S = -\sum_{i=1}^3 \sigma_{ii} \epsilon_{ii} \Omega = -\Omega (\epsilon_{xx} \sigma_{xx} + \epsilon_{yy} \sigma_{yy} + \epsilon_{zz} \sigma_{zz}) \quad (2)$$

where the σ_{ii} 's are given by Chou,⁴ and $\Omega = \sqrt{3}a^2c/4$ for the hcp crystal with lattice parameters a and c . The principal strains ϵ_{xx} , ϵ_{yy} ($=\epsilon_{xx}$), and ϵ_{zz} can be estimated from the lattice parameter variation with average solute concentration c_0 through the relation $\epsilon_{zz} = 1/c \cdot dc/dc_0$ and $\epsilon_{yy} = 1/a \cdot da/dc_0$.⁷

B. Interaction Energy Contours

The interaction energies, U_S , were computed for silver and cadmium respectively. The principal strains, ϵ_{ii} , were computed from room temperature X-ray data⁸ and are $\epsilon_{xx} = \epsilon_{yy} = 0.35$, $\epsilon_{zz} = -0.71$ for silver and $\epsilon_{xx} = \epsilon_{yy} = 0.11$, $\epsilon_{zz} = 0.27$ for cadmium, respectively. The elastic constants of zinc, silver and cadmium at room temperature⁹ were used in Equations 2 and 4. The computed results of U_S were plotted in solid contours in Figure 2. The numerical values attached to contours represent the magnitude of the energy in electron volts.

The dotted circular contours in Figure 2 represent the interaction energy in the isotropic approximation. These were computed backward from reported values of theoretical "binding energy."¹⁰ The elasticity theory breaks down in the vicinity of the dislocation center. Thus the maximum interaction energy at an arbitrary lower cut off radius of one Burgers vector has been conventionally regarded as the theoretical

"binding energy."¹⁰ The reported values of the "isotropic" computation for silver and cadmium solutes in zinc are 0.16 and 0.22 eV, respectively.⁵ The present "anisotropic" treatment gives 0.47 and 0.27 eV, respectively. The contrast between the "anisotropic" and "isotropic" contours for silver is more distinct than is the case for cadmium. These contrasts in binding energies and contours show that the "isotropic" approximation may be misleading in some cases.

The strong contrast between the shapes of "anisotropic" contours for silver and cadmium seems consistent with the strains (ϵ_{ii}) induced around each solute atom. Even though the lattice distortion around a cadmium solute atom is highly anisotropic ($\epsilon_{zz} \cong 2.5 \epsilon_{xx}$), it causes only a slight deviation from the result of the "isotropic" treatment because the principal strains are of the same sign. But for a silver solute atom there is a significant deviation because the signs of the principal strains are not the same. A silver solute atom expands the host lattice along the basal plane and shrinks along the direction perpendicular to the basal plane.⁸ Thus the "anisotropic" contours are shrunken along the z-axis in Figure 2(a) leading to a splitting of the contours into two leaves. Thus each silver solute atom has two sites of identical interaction energy with respect to the dislocation center, while each cadmium solute atom has only one site for a given interaction energy. This effect of the alternating signs of strains associated with solute atoms are also reflected in the shape of the force displacement relation in the following section.

III. THE FORCE-DISPLACEMENT RELATION

The force per unit length of dislocation, F , for an edge dislocation to glide rigidly as a whole with respect to an immobile obstacle is obtained from the relation,

$$F = -\partial U_I / \partial y \quad (5)$$

in the present coordinate system, where U_I is an appropriate interaction energy. By computing F as a function of the dislocation displacement, we can construct a diagram of the force displacement relation.

For simplicity the dislocation glide plane was set on the mid-plane between two adjacent parallel basal planes. Then the distance from the dislocation to the first two basal planes is $c/4$, and is $3c/4$ to the second nearest planes, where c is the lattice parameter along the c -axis. Any substitutional solute atoms in the first planes can approach and pass the dislocation as close as $c/4$, which is a slightly shorter distance than $b/2$ in zinc crystal. At this distance the interaction may not be expressed by the linear elasticity because of the core breakdown. However we assume that the linear elasticity is valid down to the distance of $c/4$, since we are more interested to demonstrate the effect of the anisotropy than to establish numerical values. The interaction within the core will be discussed in more detail in the next section.

The computed force-displacement relations for silver and cadmium solute atoms were plotted in Figures 3(a) and (b), respectively. The solid curves represent the "anisotropic" force for the solute atoms located in the first atomic layer below the glide plane and the dashed curves apply to the solute atoms in the second layer. The dotted curves

represent the "isotropic" forces for the first layer solute atoms, which were computed from the "isotropic" interaction energy.

The contrast between the "anisotropic" (solid lines) and "isotropic" (dotted lines) forces is more pronounced for silver than for cadmium as was anticipated from the contours in the previous section. The difference between the peak values of the "anisotropic" and "isotropic" forces is much larger for silver than for cadmium. For cadmium the "anisotropic" curve follows essentially the same trend as the "isotropic" one. For silver it shows an almost opposite behavior, especially when the horizontal distance between the dislocation and solute atom is less than one Burgers vector. The maximum peaks of the "anisotropic" and "isotropic" curves are located on the opposite sides of the vertical axis and at almost the same distance from the axis. Beside this, the "anisotropic" curve for silver has a second peak which is higher than the "isotropic" peak. This peculiar behavior of the "anisotropic" force-displacement relation is a direct result of the shape of the interaction energy contours. The solute atom occupying a lattice site in an atomic layer below the glide plane has two potential valleys, one in front and the other in the rear of the solute atom itself. Thus an edge dislocation approaching and passing the solute atom has to cross the two valleys and this causes the two peaks and two valleys in the force-displacement relation.

The solute atoms in the second atomic layer below the glide plane induce a force-displacement relation of essentially the same pattern. The values of the peak forces and their separations from the dislocation center are of one ninth of and three times of those of the first layer solute atoms.

IV. DISCUSSION

A. Core Range

Within the dislocation core, atoms are severely displaced from the regular lattice sites. The strain associated with this displacement is considered too large to be treated with linear elasticity. Furthermore, the linear elasticity equation has an inherent singularity at the origin of the coordinate system. The Peierls-Nabarro dislocation model can remove such a singularity.¹¹ But the model has been constructed by means of the linear elasticity and its application to the dislocation core region may not be justifiable.

It has been a common practice to assume that linear elasticity is valid everywhere except within the core range and to leave the core range out of the analysis. It is conceivable, however, that the most meaningful part of the dislocation-solute interaction may occur within the core. Thus Cottrell¹² suggested a correction parameter as follows. The "isotropic" interaction energy U due to the elastic size misfit is given by $U = Az/y^2 + z^2$ in the present coordinate system, where A is a constant determined by the matrix crystal and the solute atom. In the polar coordinate system through the transformation $y = r \cos \theta$ and $z = r \sin \theta$, $U = A \sin^2 \theta / r$. To remove the breakdown Cottrell introduced an adjustable parameter ρ such that $U = A \sin^2 \theta / (r + \rho)$. Stefansky and Dorn¹³ also introduced a correction parameter which is a mathematical equivalent to the Cottrell's parameter. This correction is supposed to be significant only within the core and imperceptibly small outside the core. In principle the correction parameter can be determined by comparing the measured and computed "binding" energies. However, this

procedure involves some subtlety since it is difficult to estimate the contribution from each source of interaction to the measured total interaction energy.

A more reasonable estimation of the correction parameter may come from the application of suitable interatomic potentials to the atomistic model of dislocation. Such application was already made to the dislocation interaction with vacancies and self-interstitials,¹⁴ but have yet to be extended to the interaction with foreign solute atoms. The estimation of the elastic lower limit has been done through the computation of dislocation self-energy and has turned out to be much smaller than one Burgers vector.¹⁵

B. Elastic Size Misfit

The magnitudes of the strain-components (ϵ_{ii}) associated with the solute atoms seem too high for the present linear elasticity approach to be precise. However, if one notices the rapid change in the lattice parameters⁸ of the zinc matrix as the solute content (silver and cadmium) increases, one could realize that there must be a severe deformation of the matrix by the solute atoms. One can also expect very large values of the interaction energy and forces. The deformation is so severe that these alloys (Zn-Ag and Zn-Cd) do not seem to remain as a single phase even at a small solute content. These solute atoms have, in fact, very limited solubilities in zinc, only 5 and 1.7 atomic percent for silver and cadmium respectively.¹⁶

C. Results and Implication

The numerical results in this report may be very difficult to confirm experimentally. The only available experimental "binding energy" for a cadmium solute atom in zinc was obtained using an internal friction method and is 0.07 eV^5 . The present computation gives 0.27 eV . However, the "empirical value" itself was obtained through an indirect theoretical reference,¹⁷ from the internal friction data; hence its precision is uncertain. A qualitative confirmation of the "anisotropic" feature for silver solute may be a very difficult task, also. Current experimental techniques are not very sensitive to the variation in the shapes of the force-displacement diagram or the interaction energy contours.

The "anisotropic" treatment does not induce any extra difficulty in the theoretical analysis of the solute-dislocation interaction for the case of cadmium. It causes simply a numerical amplification of the force-displacement diagram. However, for the case of silver, the existence of the secondary peak in the force-displacement diagram presents some additional complications in the dislocation motion. Consider the thermally activated glide of a dislocation through a distribution of the silver solute atoms in the zinc matrix under the influence of an external force. The dislocation may have to be activated twice to overcome one of the solute atoms which are pinning the dislocation, even if the activation energy for the primary peak is much larger than for the secondary peak. The dislocation may jump to an intermediate configuration of stable equilibrium between the two peaks of the force-displacement diagram after the initial activation. Thus in a certain configuration of the dislocation and solute atoms along the dislocation,

the strength of some of the solute atoms as obstacles to the dislocation glide may be characterized by the secondary peak rather than the primary peak. If, however, one of the two peaks is much higher than the other, these additional complications may be safely ignored.

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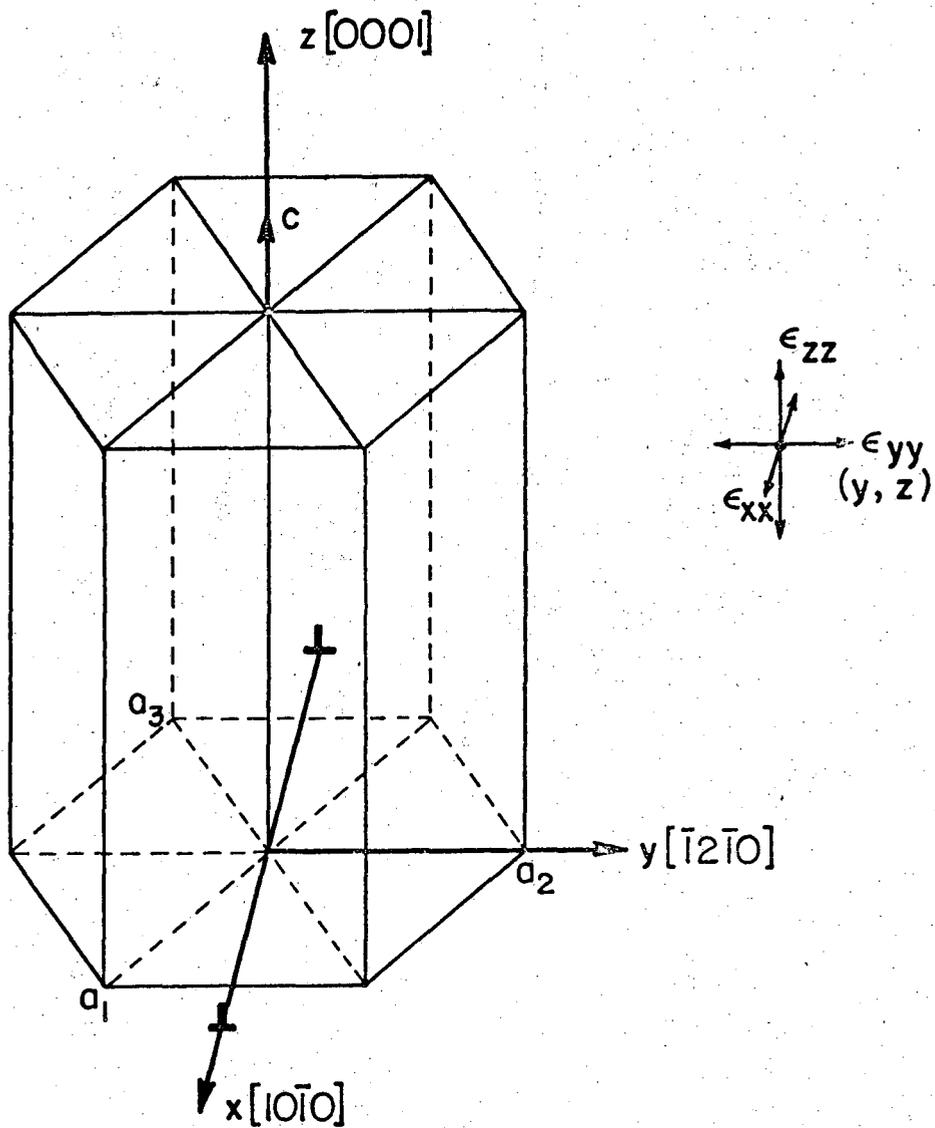
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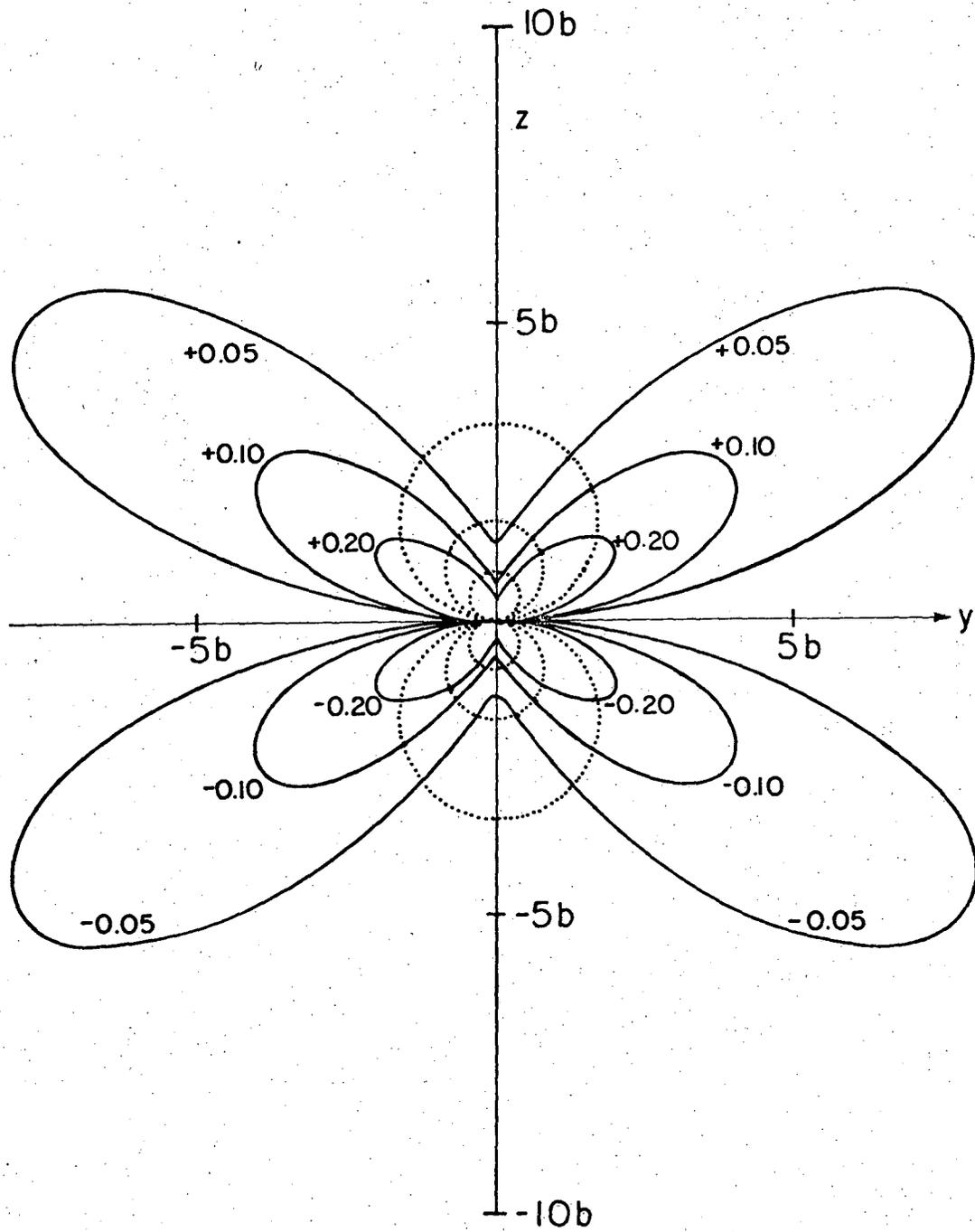
FIGURE CAPTIONS

- Fig. 1. Cartesian coordinate system in hcp crystal.
- Fig. 2. Interaction energy contours (a) for Ag and (b) for Cd in Zn, Solid lines for "anisotropic" and dotted lines for "isotropic" contours.
- Fig. 3. Force-displacement diagrams (a) for Ag and (b) for Cd. Solid and dashed lines for "anisotropic" diagram for solute atoms in the first and second nearest planes below the dislocation. Dotted lines for "isotropic" diagram for the first layer solute atoms.



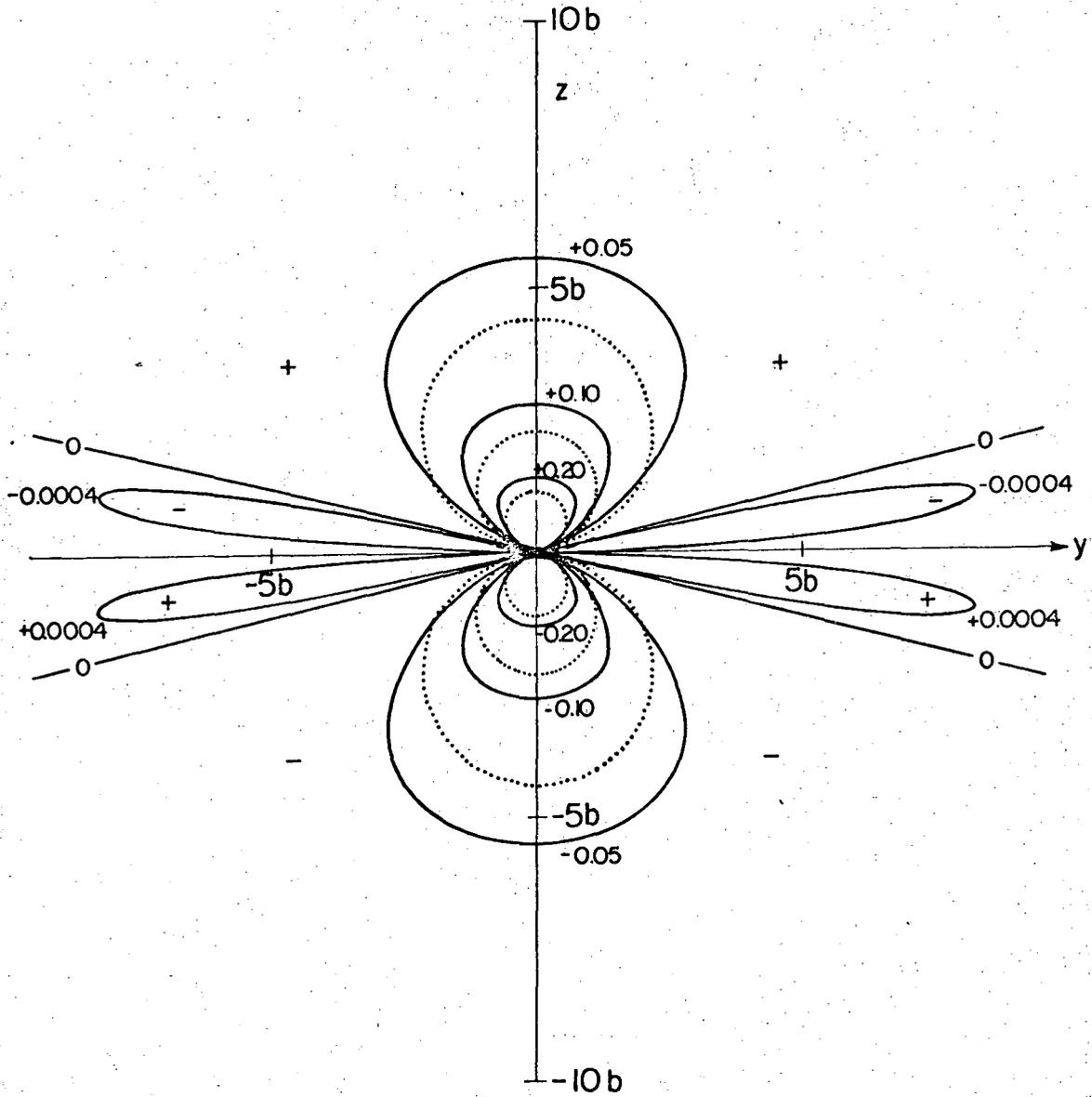
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Figure 1



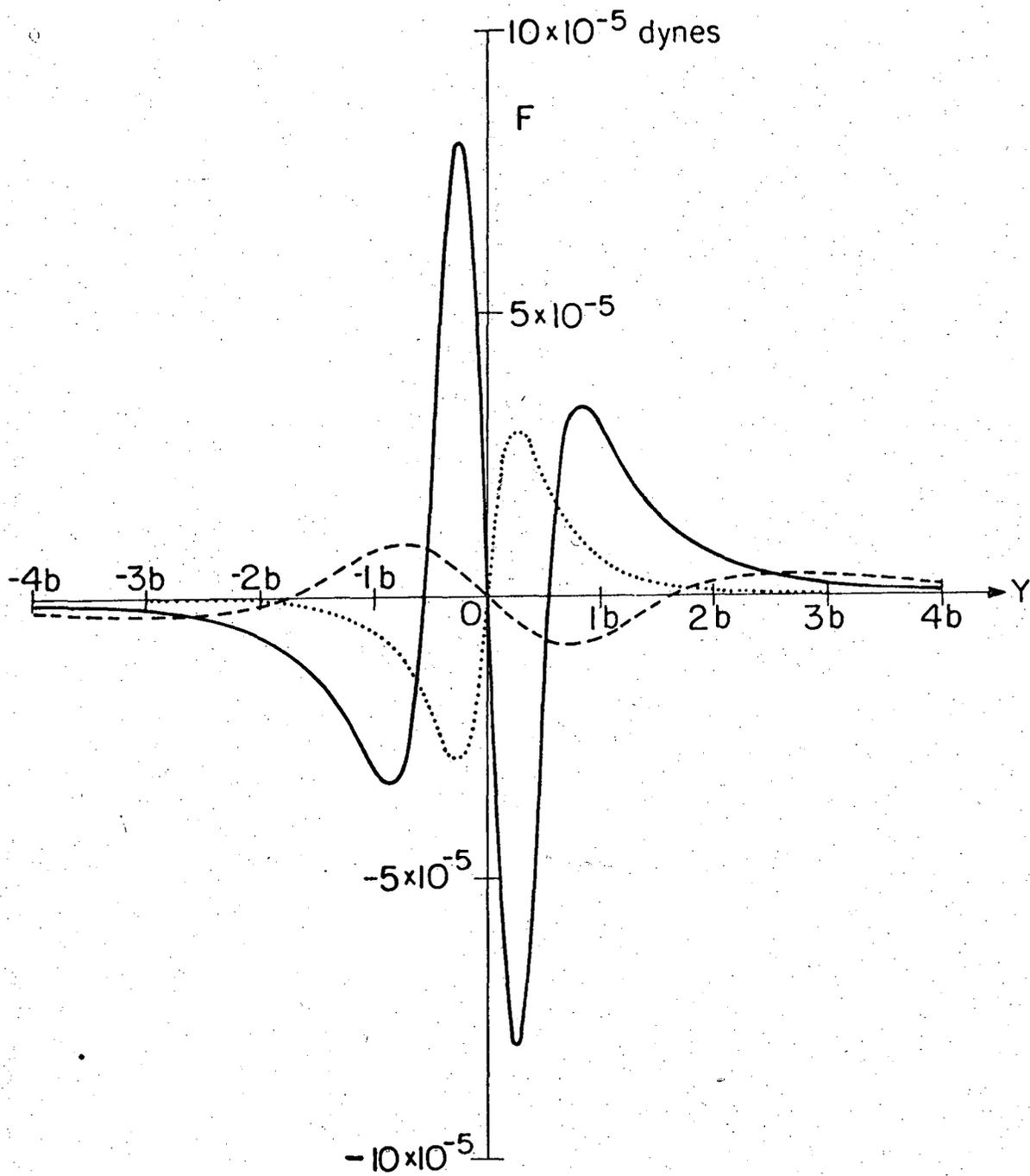
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Figure 2(a)



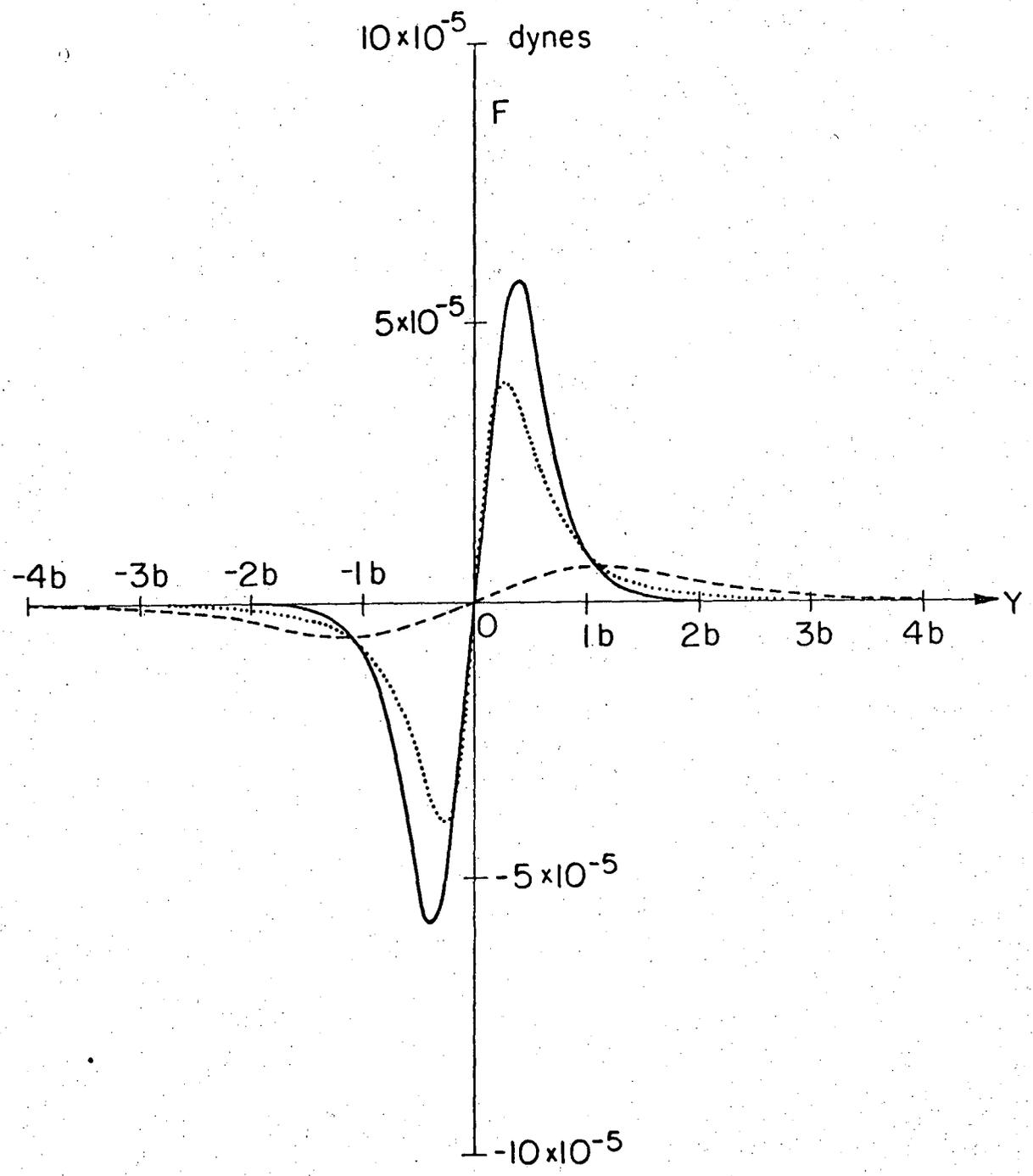
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Figure 2(b)



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Figure 3(a)



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Figure 3(b)

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